Naval Ocean Research and Development Activity
August 1988 Report 239

AD-A203 781

Improvements to the Data Selection Algorithms in the Optimum Thermal Interpolation System (OTIS)

Patricia A. Phoebus
Ocean Sensing and Prediction Division
Ocean Science Directorate

Foreword

The Navy's mission is highly dependent upon our ability to provide a timely and accurate depiction of ocean thermal structure. However, because of the vastness of the world's oceans, the amount of data available to the Navy's operational oceanographic centers is limited, at best. Thus, it is absolutely essential to make optimum use of these observations. Therefore, the Fleet Numerical Oceanography Center is developing and testing an improved thermal analysis system, the Optimum Thermal Interpolation System (OTIS).

The Naval Ocean Research and Development Activity has been very active in the development of this new product, and our scientists have made many suggestions that have resulted in an improved analysis. Particular attention has been paid to properly utilizing the available data. This report focuses on changes made to the original data selection procedures in OTIS to assure that the resulting analysis is more representative of the true ocean thermal structure, and thereby to provide the Fleet with a more useful environmental product.

William B Moseley

W. B. Moseley
Technical Director

A. C. Esau, Captain, USN
Commanding Officer

Executive Summary

The Fleet Numerical Oceanography Center (FNOC) provides daily analyses of the three-dimensional ocean thermal structure both to the Fleet and to regional naval oceanography centers around the world. These analyses are made for both global and regional areas at resolutions as small as 20 km in some regions. FNOC is planning to update these products very soon with an improved analysis based on the widely accepted methodology of optimum interpolation. This system, the Optimum Interpolation Analysis System (OTIS), is expected to provide a more accurate representation of the three-dimensional ocean thermal structure.

As with any new system, extensive development, testing, and evaluation has been done. Many modifications were made to the original design. While studying the impact of multichannel sea surface temperature data on the analysis of the ocean's sea surface temperature, several errors were uncovered in the data selection algorithms. These errors were also apparent in the subsurface analyses.

Since it is not feasible to use all observations to estimate the temperature at any one location, optimum interpolation chooses a subset of the available data using correlation scales that are representative of the spatial and temporal scales of the ocean features to be analyzed. Practically speaking, observations that are closer to the analysis point and that were taken more recently are the observations most highly correlated with the analysis point.

Generally, all data within a certain cutoff correlation range are collected at an analysis point. Within OTIS, the designated search area was too small and did not correspond to the shape of the spatial correlation function. As a result, observations more highly correlated than those actually collected were excluded from consideration. Furthermore, limited computer resources forced artificial cutoffs to be placed on the collection of observations. The method of data storage resulted in frequently excluding data that were the most highly correlated with the analysis point, while gathering observations farther to the south.

From the initial set of collected data, a few of the most highly correlated reports will be selected as input to the analysis. Only these selected observations will have any effect on the analyzed temperature at that particular location. If the set of collected data does not include the most highly correlated observations, then the selection process cannot choose the most appropriate data for the analysis. Also, if the selected observations are skewed to the south, then biases in the resulting temperature analyses can be produced.

Errors in the data selection procedure were corrected; at the same time the data selection software was redesigned to make more efficient use of the available resources. Correctly selecting the optimum data for the analysis at each point resulted in significant changes in the analyzed temperature fields, and noticeable improvements in the representation of the three-dimensional thermal structure of the ocean.

Acknowledgments

Others must be given credit for assisting with this work. Dr. Ted Bennett of NORDA's Ocean Hydrodynamics/Thermodynamics Branch provided valuable programming support through his contract with Mr. Lance Reidlinger of Planning Systems Incorporated. Without their help, this experiment would have taken much longer to complete. Mr. Mike Clancy (FNOC) provided his insight and perception as we discussed potential solutions to the identified problems and, along with Mr. Ken Pollak (FNOC), supplied time and assistance during the testing of these modifications. They were directly responsible for identifying certain oversights that were made in the initial design of the software.

This research was supported by the Chief of Naval Operations (OP-096) under Program Element 63704N, Satellite Applications and Technology, Mr. A. E. Pressman, Program Manager, and by the Space and Naval Warfare Systems Command under Program Element 63207N, Air-Ocean Prediction Capt. J. Jensen, Program Manager.

Contents

Improvements to the Data Selection Algorithms in the Optimum Thermal Interpolation System (OTIS)

I. Introduction

The theory of optimum interpolation was first applied by Gandin (1963) to the analysis of atmospheric parameters. Over the years, optimum interpolation has been adapted for use at many of the world's meteorological forecast and research centers (Schlatter, 1975; Rutherford, 1976; McPherson et al., 1979; Lorenc, 1981; Daley et al., 1985; Baker et al., 1987; Barker et al., 1988). Application of optimum interpolation techniques to the analysis of oceanographic parameters received some early attention (Bretherton et al., 1976; Freeland and Gould, 1976; White, 1977), and has recently been utilized for data analysis and assimilation by Carter and Robinson (1981), Roemmich (1983), Robinson and Leslie (1985), and McWilliams et al. (1986). The Navy's Fleet Numerical Oceanography Center (FNOC) is evaluating the first operational three-dimensional ocean thermal analysis system based on optimum interpolation theory. This analysis scheme is called the Optimum Thermal Interpolation System (OTIS).

The Naval Ocean Research and Development Activity (NORDA) has played a major role in the development of that system, which is a three-dimensional global univariate analysis. Work is currently underway at FNOC and NORDA to add regional capabilities to OTIS. In addition, a sea surface temperature (SST) version of OTIS (SST-OTIS) has been developed by NORDA's Remote Sensing Branch in order to evaluate the proper role of satellite multichannel sea surface temperature (MCSST) data in higher-resolution thermal analyses. The SST-OTIS is nearly identical in function to the three-dimensional version of OTIS. One major difference is that OTIS averages the MCSST data to create "superobs," which are then input to the analysis. The SST-OTIS utilizes all available MCSST data individually for analyzing mesoscale fronts and eddies. Also, because of its higher resolution grid and larger data handling requirements, the SST-OTIS was developed to run on FNOC's supercomputer—the Control Data Corporation Cyber 205.

Because of the many similarities between OTIS and the SST-OTIS, problems that arose during the development of the SST-OTIS were usually problems in OTIS, as well. The simpler design of the SST-OTIS made it an excellent framework for testing and evaluating techniques that were applicable to both systems. In particular, the SST-OTIS has the capability to do an analysis at only one or two points. Since the analyses at each grid point are independent of one another, this capability is a useful and efficient way to study in detail the various algorithms that comprise the analysis. As a result, major improvements have been made in the areas of data selection and quality control. Only the former will be addressed in this report. The quality control algorithms will be discussed in a separate report (Phoebus, 1988, in preparation).

In order to address the problem of data selection, a brief explanation of optimum interpolation is presented. Then, the original data selection algorithms in OTIS are discussed. Some of the problems with these techniques are illustrated, and the steps taken to improve them are detailed. The impact of these changes is discussed in section V, the implementation of the corrections explained in section VI, and suggestions for further improvements are outlined in section VII.

II. Background

The basic optimum interpolation methodology is discussed in various papers (Alaka and Elvander, 1972; Bergman, 1979; Lorenc, 1981). The particular equations and techniques applied in OTIS are described in detail by Clancy et al. (1988). Optimum interpolation produces an estimate of a variable at a grid point such that the analysis error is minimized in a least-squares sense. The analyzed variable is usually computed in the form of a correction to a first-guess field. That correction is calculated as a linear combination of weighted anomalies, where an anomaly is simply the deviation of an observation from the background field. Therefore, the first step is to choose the appropriate observations.

In OTIS, the analyzed temperature at a particular grid point k is given by

$$T_k^a = T_k^c + \sum_{i=1}^{N} \alpha_{ki} \, (T_i^o - T_i^c) + \beta_k \, (T_k^p - T_k^c), \tag{1}$$

where T_k^c is the first-guess temperature at the grid point (generally climatology), T_i^c is the first guess interpolated to the location of observation i, T_i^0 is the temperature of the i^{th} observation, and α_{ki} is the weight calculated for each observation. The last term represents the contribution made by the Thermal Ocean Prediction System (TOPS) mixed-layer model's predicted temperature, and is not critical to this discussion. Thus, to simplify the equations, assume a model prediction is not available. Then equation (1) becomes

$$T_k^a = T_k^c + \sum_{i=1}^{N} \alpha_{ki} \, (T_i^0 - T_i^c). \qquad (2)$$

The weights α_{ki}, which will minimize the analysis error at grid point k, are obtained by solving the set of linear equations

$$\eta_{ki} = \sum_{j=1}^{N} (\eta_{ij} + \delta_{ij} \lambda_i^0) \; \alpha_{ki}, \; for \; i = 1,2,\ldots N, \qquad (3)$$

where η_{ij} is the autocorrelation between observations i and j, η_{ki} is the autocorrelation between observation i and the estimated value at the grid point k, λ_i^0 is the noise-to-signal ratio for observation i, and δ_{ij} is the Kronecker delta function, defined as

$$\begin{aligned} \delta_{ij} &= 1 \quad for \; i = j \\ \delta_{ij} &= 0 \quad for \; i \neq j. \end{aligned} \qquad (4)$$

The autocorrelation function η_{ij} between any two temperatures at locations i and j is chosen to be the Gaussian function

$$\eta_{ij} = exp \left[- \left(\frac{\Delta X_{ij}}{AX_k} \right)^2 - \left(\frac{\Delta Y_{ij}}{BY_k} \right)^2 - \left(\frac{\Delta \tau_{ij}}{CT_k} \right)^2 \right], (5)$$

where AX_k, BY_k, CT_k are the E-W, N-S, and time correlation scales at grid point k, and ΔX_{ij}, ΔY_{ij}, $\Delta \tau_{ij}$ represent the E-W, N-S, and time separation of the observations at locations i and j. The same function is used to calculate η_{ki}, where k represents the grid point location and the age of the estimated temperature at location k is 0.

To be truly optimum, all observations within the entire data set would be input into equation (3) and the matrix problem would be solved at every grid point. Since solving such a large matrix is not practical because of limited computer resources, the techniques used in OTIS and other optimum interpolation analyses generally use only a few observations for the analysis at any one point. In fact, even if resources were unlimited, a case can still be made for not including all observations in the analysis at every grid point. Most data analysts agree that some observations are so poorly correlated with the analyzed variable at a particular grid point that the weight given to that observation would be negligible (McPherson, 1980). For example, an observation taken in the Sargasso Sea contains little useful information about the temperature off Nova Scotia.

Therefore, if only a subset of the available data is allowed to influence the analysis at a particular point, then the problem becomes how to define which observations should comprise that subset, and how large the subset should be. Ideally, if only a limited number of observations can be selected, then the preferred observations are those that provide the most pertinent and most independent information about the analyzed variable at the grid point in question.

The independence of the selected data can be improved in several ways. Forcing data to be selected from various sources and in various directions from the grid point has been used to prevent the selection of redundant data (Phoebus, 1985). The use of "superobs" (Lorenc, 1981), where closely spaced data are combined into one observation prior to the data selection, is common and is used in OTIS for the MCSST data. Duplicate observations, taken by the same platform but reported twice, are frequently present in the global data sets and should be removed. Redundant information is also present in data from platforms that report with great frequency, such as buoys. Such data can be filtered prior to the selection of observations.

The choice of the most pertinent data is more difficult to define. Several approaches are widely used to select the "best" observations (Barker and Rosmond, 1985). One choice would be to use the distance from the grid point and select the closest observations. A variation of this method uses distance and direction in order to force the data to be equally distributed about the grid point, if possible. A third method would be to use covariances to select the observations that are the most highly correlated with the estimated value at the grid point in question. Even more complex criteria may involve both covariances and direction (Phoebus, 1985).

Because OTIS uses spatially noncircular correlation functions, which are also functions of time, the covariance method is the one chosen for this application. Use of the covariance method allows OTIS to give higher consideration to more recent observations and to observations that lie across, not along, the typical temperature gradients of the ocean. If the spatial correlation function is circular and if all of the observations are taken at the same time, then this method is equivalent to the distance method.

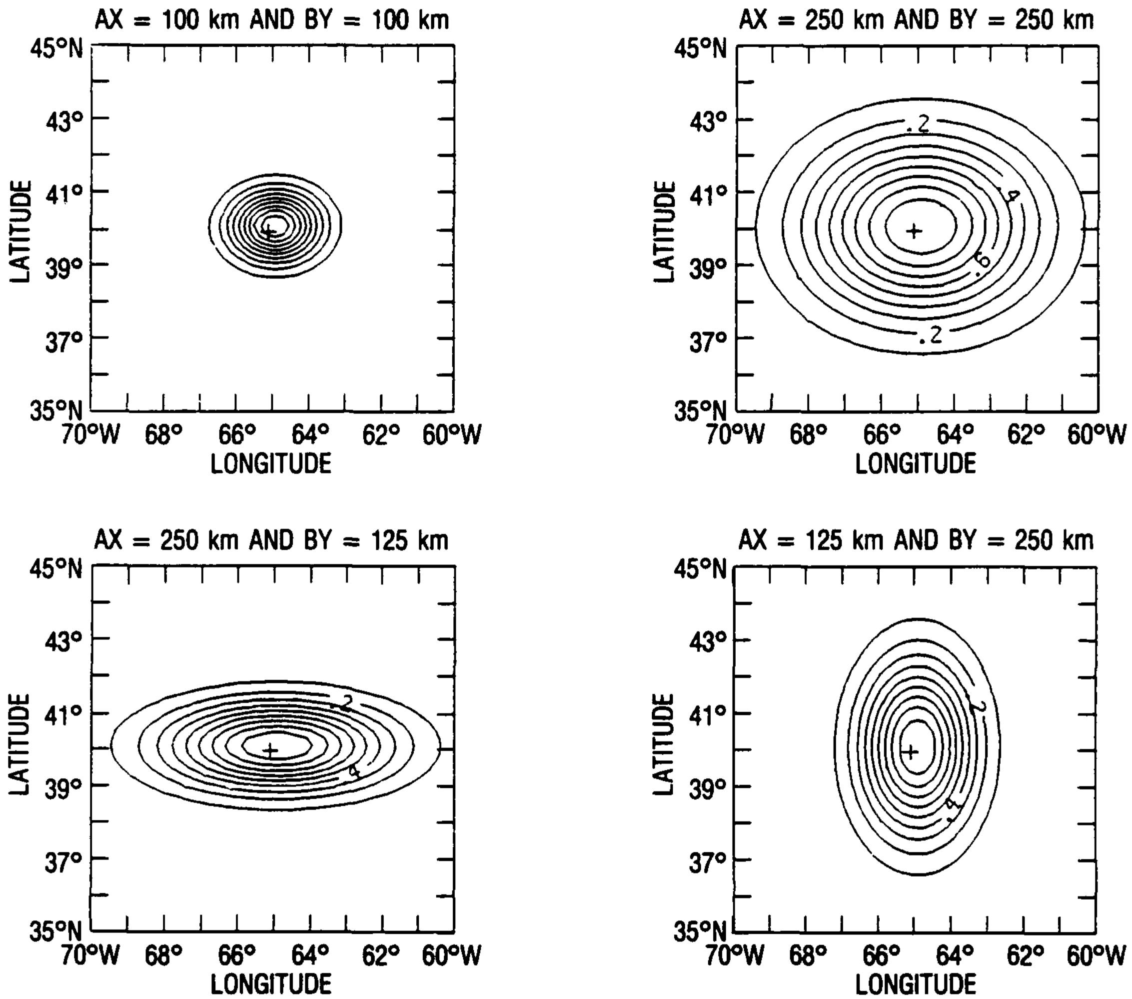

Figure 1. Shape of the Gaussian spatial correlation function, given various values for the east-west (AX) and north-south (BY) correlation scales. Contours represent the correlation of an observation at a particular location with the grid point value at the center of the figure. Correlations are contoured from 0.1 to 0.9, with an interval of 0.1.

III. Data Selection Algorithm

Before particular observations are collected for an analysis at a grid point, an area of influence is defined around the grid point so that only a subset of the data must be searched to find the most highly correlated observations. Using the covariance method, this search area is defined as a function of the spatial correlation scales that are appropriate for the grid area under consideration.

In OTIS, the spatial correlation function has the form of equation (5), assuming $\Delta\tau_{ij} = 0$, that is,

$$\eta^s_{ij} = exp\left[- \left(\frac{\Delta X_{ij}}{AX_k}\right)^2 - \left(\frac{\Delta Y_{ij}}{BY_k}\right)^2 \right], \qquad (6)$$

where AX_k and BY_k are the correlation scales in the E-W and N-S directions, respectively, and ΔY_{ij} and ΔX_{ij} are the latitudinal and longitudinal differences between two points, converted to distances in kilometers. If one of these points is the grid point, then the correlation function can be thought of schematically as a set of concentric geometric figures centered at the grid point location. If AX_k and BY_k are equal, then those figures are circles; if $AX_k > BY_k$, or vice versa, then the figures are elliptical. Figure 1 illustrates the shape of the spatial correlation function for some typical correlation scales used in high-resolution ocean thermal analysis.

The area surrounding the grid point will be searched for data within a latitude/longitude box centered at the grid point and whose sides are one correlation distance from the grid point (Fig. 2). More explicitly, the areal limits are the latitudes and longitudes that result in $|\Delta X_{ik}| = AX_k$ and $|\Delta Y_{kj}| = BY_k$. Along the sides of this rectangle, the maximum correlation is equal to e^{-1}, or about 0.37. However, because the

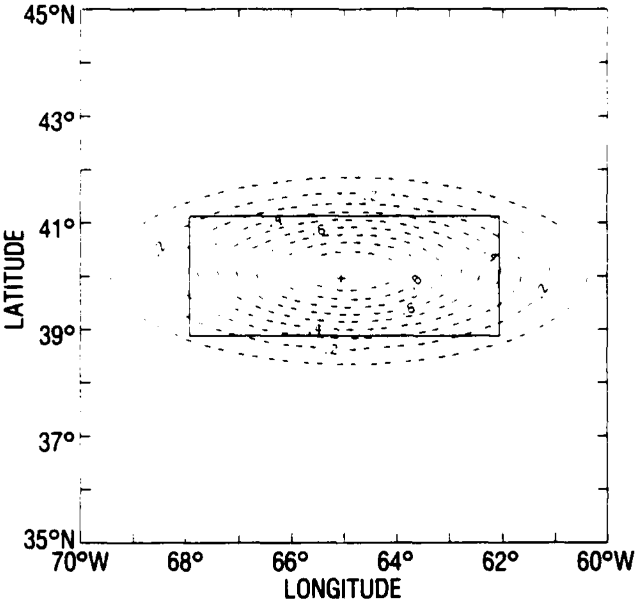

Figure 2. The rectangular area is the area to be searched for data for the analysis at the center grid point, given a search area defined as one correlation length in both the x and y directions from the grid point. The set of concentric ellipses represent the spatial correlation function at 0.1 value increments for the case where the east-west correlation scale is 250 km and the north-south scale is 125 km.

shape of the correlation function is not rectangular, observations in the corner regions of the search area have correlations less than 0.37. Therefore, the potential is created for including data from the corners whose correlations are significantly smaller than the correlations of observations that are excluded due north, south, east, and west of the grid point. Nevertheless, this is the area from which data are currently collected.

The number of observations selected for the analysis is limited to 15. The specification of this number is somewhat arbitrary, although the experience of others (McPherson, 1980; Schlatter, 1975) has shown that most of the information about the correction to be made at a grid point is contained in relatively few observations. Indeed, even for three-dimensional multivariate applications, fewer than 35 observations are normally selected (Carr, 1987). The exception is the so-called "volume" method, described by Lorenc (1981) and used by FNOC (Barker et al., 1988) and others for meteorological applications. In this method, all observations within a large three-dimensional volume are included in the analysis at every grid point within the volume. Such an approach cannot be considered at this time because of the limited computer resources currently available to OTIS.

To select the 15 "best" observations, the total correlation between the grid point and each data point in the specified search area must be calculated using the correlation function defined in equation (5), where the location of point j is taken to be the grid point k, and $\Delta\tau_{ik}$ is the age of the observation in hours. The difference between this function and the function given in equation (6) is that the time correlation has been included. Because of the nature of the exponential function, the total correlation can be thought of as the spatial correlation multiplied by the time correlation η^{τ}_{ij}.

$$\eta_{ik} = \eta^{s}_{ik} * \eta^{\tau}_{ik} = \eta^{s}_{ik} * exp\left[-\left(\frac{\Delta\tau_{ik}}{CT_k}\right)^2\right], \qquad (7)$$

where the symbol * represents multiplication. Since the time correlation is always less than or equal to 1 (Fig. 3), an older observation has a smaller total correlation with the estimated value at the grid point than does a more recent observation taken at the same location.

Once all the observations within the search area have been collected, and their correlations computed, they are sorted in order of their total correlation with the estimated value at the grid point. The 15 most highly correlated are then saved for input to the analysis. If less than 15 observations are found within the search area, then all of those observations will influence the analysis at the grid point in question.

IV. Discussion Of Research Problem

To facilitate the collection of the observations in the search area at each grid point, both the data and the grid points are sorted in order of increasing latitude from south to north. In addition, locations at the same latitude are further sorted by longitude from east to

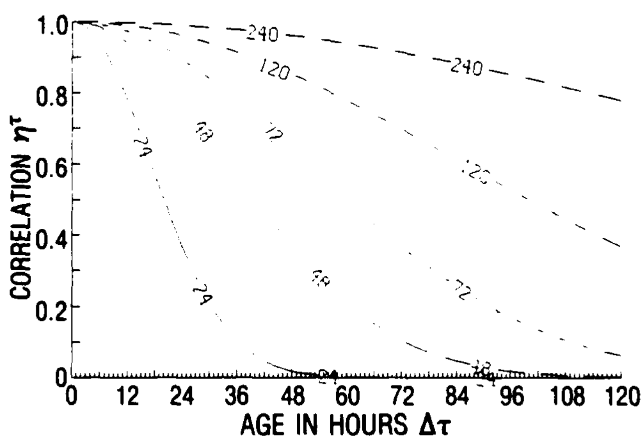

Figure 3. The contribution of the time correlation function as a function of the age of the observation. The five curves represent the rate of decay with age for five different time correlation scales, from 24 to 240 hours.

west. For regional applications, both data positions and grid points are tagged with a water mass indicator. Only data within the same water mass as the grid point are collected (STX, 1987). Such preparations reduce the amount of data that must be contained in central memory at any one time and reduce the amount of time spent performing the data search.

Because of limited computer resources and because arrays within computer programs must be assigned some finite dimension, the number of observations collected within the search area of one grid point must be limited. At the time of these experiments, OTIS set that limit at 80 observations per point. Herein lies the potential problem—the search area may contain more than 80 observations; thus, data could possibly be excluded during the data collection process.

The data collection proceeds through the search area from south to north. Since the data are sorted in order of increasing latitude, if more than 80 observations are within the specified search area of the grid point, only the 80 southernmost observations would be collected. There is no assurance that these 80 would contain the 15 data points most highly correlated with the grid point. Nevertheless, the 15 would be chosen from this group. Thus, the data selected for the analysis are probably not the most appropriate data. Additionally, since the chosen data are likely to be skewed to the south of the grid point, there is a very real possibility of generating biases in the resulting temperature analyses.

This problem first came to attention during the development of the SST-OTIS. The initial assumption was that the requirements for the data search on a high-resolution grid would be increased because of the abundance of high-density MCSST data that would be available (recall that OTIS prefilters this data). Tests were run on the FNOC 125 x 125 Gulf Stream grid to decide what those requirements might be. As a result, an upper limit of 700 observations was necessary to guarantee that all of the data within the search area were given consideration in the data selection process. However, this result could not clearly be translated to the hemispheric three-dimensional OTIS because of the differences in the data sets, the grid resolutions, and the specified spatial correlation scales. But it did suggest that there was very likely a problem in OTIS as well.

To initially test this hypothesis, the SST-OTIS was used to do a surface analysis on the FNOC northern hemisphere grid, utilizing the same statistics that were specified in OTIS, but allowing up to 700 observations to be collected at each grid point. The result of this test is shown in Figure 4, which is a contour plot of the number of observations collected per point on 3 August 1987. Notice that large areas of the grid found more than 80 reports per point.

Upon examination of the original OTIS software, a diagnostic message was discovered that indicated when 80 observations had been collected. But the message was in the wrong place and never produced the appropriate warning to those monitoring the performance of OTIS. To find out the extent of the problem, the issue had to be investigated within the full framework of OTIS.

The entire OTIS system had to be executed exactly as it was implemented at FNOC, which meant using the same correlation scales and the same search areas. Most importantly, the data included in these experiments were required to have the same time constraints as the data in the operational OTIS would have. At the surface, that required 60 hours of MCSST data, 48 hours of XBT data, and 72 hours of ship and buoy data. Because of the larger time scales in the deeper ocean, up to 60 days of XBT observations are included in the subsurface analyses. These periods are commonly referred to as the data windows.

To determine what a suitable upper limit for data collection might be, array sizes within the OTIS program had to be increased. As the array sizes increase, so does the central memory required for the execution of OTIS. Since the larger memory requested greatly exceeded FNOC specifications for operational products, special permission had to be obtained from FNOC before these experiments could begin.

With assistance from NORDA's Ocean Hydrodynamics/Thermodynamics Branch, who has primary responsibility for three-dimensional ocean thermal analyses, several different tests were designed with limits of 80, 160 and, finally, 240 observations per search area. Each set of tests was performed on several different days (see Table 1) to make the results less dependent on any one particular data set. Output was produced for both surface data and for subsurface data at the selected level of 400 m.

As these experiments began, additional restrictions discovered within OTIS further inhibited the

Table 1. Central memory and central processor time required for each of the OTIS experiments.

OTIS COMPUTER RESOURCE REQUIREMENTS Data Collection Experiments			
Number of Obs Collected	Central Memory (Octal words)	Execution Time (CPU Seconds)	Date of Test
80	176300	519.0	9-03-87
80	176300	498.5	9-04-87
80	176300	484.0	9-09-87
80	174400	487.1	9-14-87
160	216300	562.4	9-03-87
160	216300	545.5	9-04-87
160	216300	518.1	9-09-87
240	236100	527.7	9-04-87
240	236100	523.0	9-09-87
240	236100	537.0	9-10-87
240	234200	524.8	9-14-87

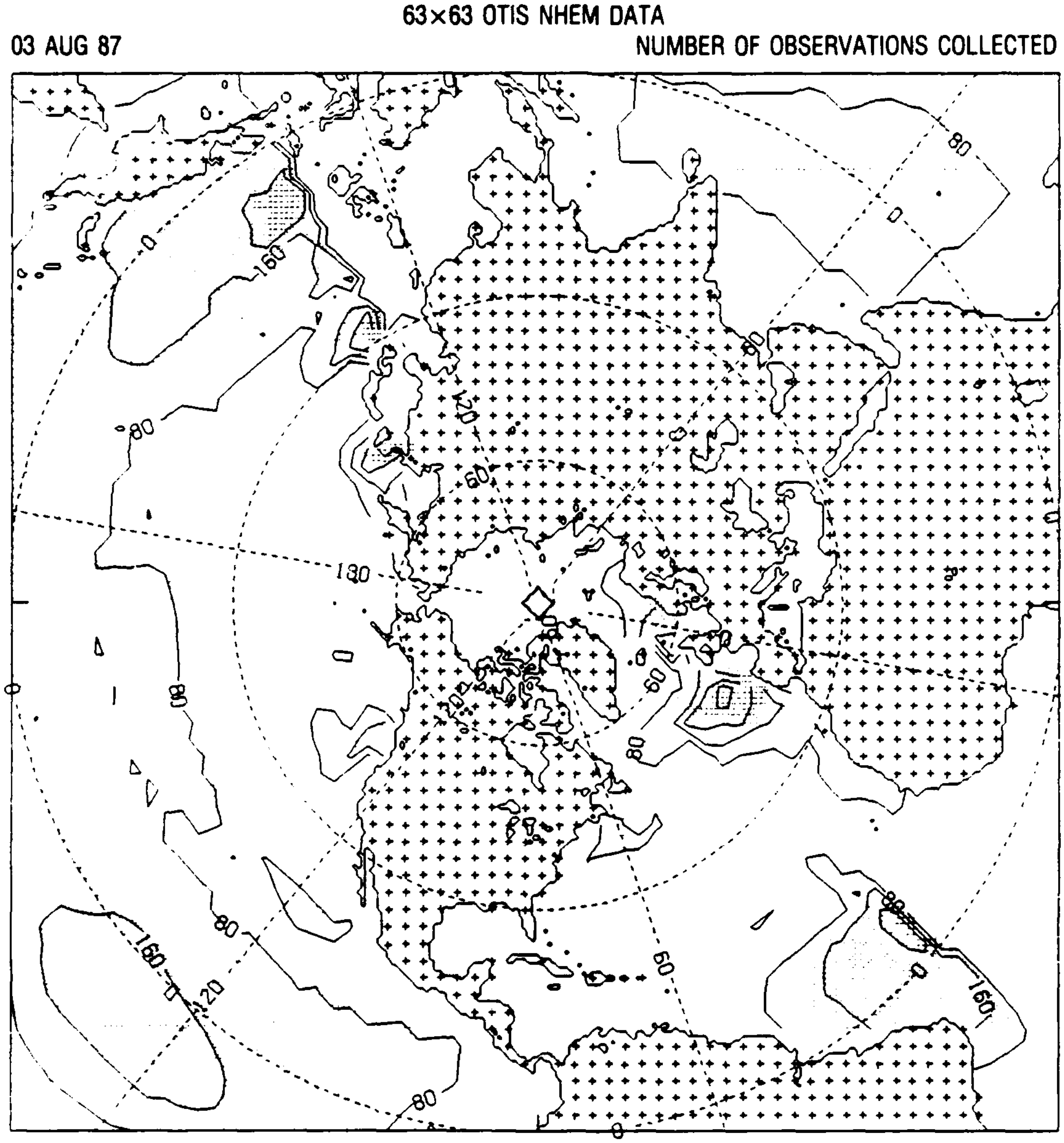

Figure 4. Shaded areas indicate regions where more than 80 observations were found within the search areas of the grid points in those regions. Contours are for every 80 observations.

appropriate selection of data. In addition to the limit of 80 total observations, constraints were placed on each data type. As a result, no more than 20 XBT (expendable bathythermograph) reports, 30 ship or buoy reports, and 30 MCSST superobs could be collected at the surface. To require that some data be collected from each of the separate data sources is admirable and desirable. But as implemented in OTIS, this requirement only placed further restrictions on the data search. For example, if only ship data were available and there were 200 individual reports in the search area, only 30 would be collected, not 80, which certainly does not fully utilize all available resources. Furthermore, the best solution for achieving the desired goal is to assure that all data within range are collected. Collecting all data automatically guarantees that each report from every available source will receive full consideration in the selection process. Therefore, all limits placed on individual data types were removed.

V. Results

The results of these experiments are shown in the form of histograms, and are broken down into several different categories—all surface data, only surface XBTs, only ships and buoys, only MCSSTs, and all subsurface data. This way, the type of data most often excluded could be determined. The abscissa of each histogram is the number of observations collected. The ordinate is the number of grid points finding that number of observations. Because of the large range in the ordinate values, they are plotted using a

logarithmic scale. While this method makes it necessary to exclude the case of 0 occurrences, it does allow the large peaks that occur at the data limits to be shown. The results for 14 September 1987 are shown in Figures 5 through 22. The results for the other days were similar.

The total number of grid points on the FNOC 63 x 63 hemispheric grid is 3969. Of these, 1215 are over land, leaving 1747 grid points where an analysis may be done. In Figure 5, which depicts all surface data, notice that 81 grid points found no observations at all, while 1131 grid points collected the maximum allowable number—in this case, 80. That is, roughly 63% of the grid points excluded some observations during the data collection procedure. When broken down by data type at the surface, the impact of the individual limits can be evaluated. For example, very few points found more than 20 XBTs (Fig. 6), while many grid points found more than 30 ship and buoy observations (Fig. 7) or more than 30 MCSST superobs (Fig. 8).

While there is only XBT data at subsurface levels, the time scales and data windows are also considerably longer. Thus, much older data is used for the analysis here than at the surface. Because of the larger time windows, it was suspected that data were also being omitted at subsurface levels. The results presented in Figure 9 verify that is indeed the case. At 400 m, the problem is not as extreme as at the surface, but 41% of the grid points still did not gather all the available data.

The limit on the number of observations collected was increased, first to 160, then to 240. At 160, the same problems were evident, with many points excluding data. Only when the limit was increased to 240 did the number of grid points exceeding the limit become reasonably small. At the surface (Fig. 10), 2% of the grid points collected 240 data points, while at subsurface (Fig. 14), only 6 points found that number. When the surface data are broken down by data type (Figs. 11-13), only ship and buoy data were being excluded at the surface.

As stated earlier, the implication of not considering all of the observations within correlation range of the grid point is that the data influencing the analysis at a particular point are not the data containing the most information about the temperatures at that point. Therefore, the impact of this error on the analysis must be evaluated. Plots of analyzed temperatures at 0 m are shown for the case of 14 September 1987, both collecting 80 observations per point (Fig. 15) and 240 observations per point (Fig. 16). (The unrealistic gradient in the Atlantic Ocean off the west coast of Africa is a result of the drastic change in the east-west correlation scale at 30°W, from 1500 km to 250 km. This problem has since been identified and corrected in OTIS by using smoothly varying correlation scales.)

The temperature changes due to the selection of more correlated data are not apparent until difference maps are studied. The analyzed temperature fields produced with an 80-observation limit are subtracted from the fields produced collecting 240 observations. The difference maps for the surface are shown as two plots, one for positive differences and one for negative differences, each contoured at intervals of 0.5°C. Figure 17 shows a few isolated areas, mostly in the tropics, where the temperature was at least 0.5°C warmer when more data were included. The areas where the surface temperature decreased by at least 0.5°C are much more widespread (Fig. 18). The maximum temperature change in both plots was less than 1.5°C.

Results for the subsurface analyses are represented by the 400-m analysis level. The analyzed temperature fields at 400 m on 14 September 1987 are shown for both the 80-observation case (Fig. 19) and the 240-observation case (Fig. 20). As before, both positive and negative difference maps are computed and contoured at 0.5°C intervals. Figures 21 and 22 illustrate the typical temperature differences observed at 400 m. Increasing the number of observations collected generally resulted in warmer temperatures, with some differences larger than 2.0°C. Again, these areas are mainly in the tropics, where the spatial correlation scales specified in OTIS are larger (Table 2).

These areas are exactly where the largest changes are expected. Larger correlations scales imply larger search areas. As the size of the search area increases, data are more likely to be excluded because of the limitations placed on the number of observations that can be stored for any one point. The correlation scales are largest in the tropics and in the middle and eastern sides of the major ocean basins. The temperature changes observed are compatible with these assumptions. Only the compilation of long-term statistics on the performance of OTIS will demonstrate that the analysis in these areas has been improved due to the inclusion of more appropriate data, but it is hard to imagine that the end result could be anything but positive.

VI. Implementation of Corrections

The major recommendation resulting from this work is obvious—increase the array dimensions to allow all of the available data within the specified correlation range of a grid point to receive equal consideration as input to the analysis. The implementation of that idea is more complicated, as illustrated in Table 1. While the execution time did not increase significantly, allowing 240 observations to be collected increased the central memory requirements from around 176000 octal words to 236000 octal words. This increase far exceeds the limits on central memory under which operational products are constrained to run at FNOC (on the computer in question). Therefore, to increase the number of observations collected, which obviously

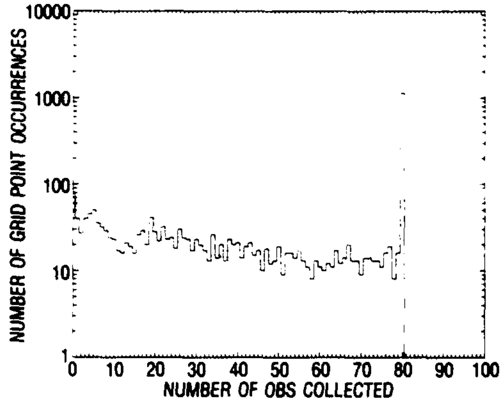

Figure 5. Histogram of all surface data collected on 14 September 1987. Each grid point was limited to no more than 80 observations, which explains the peak at 80.

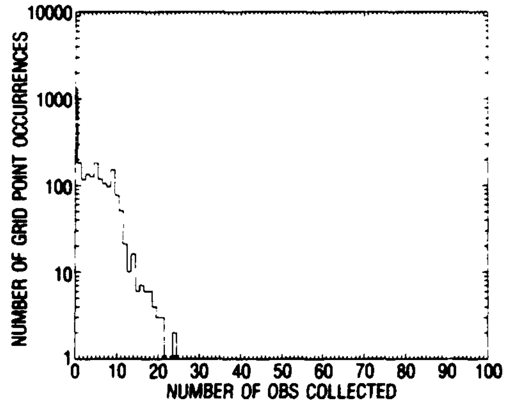

Figure 6. Histogram of all surface XBT data collected on 14 September 1987. Note that over 1000 grid points found no XBTs within their search areas. In practice, each grid point was limited to no more than 20 XBTs.

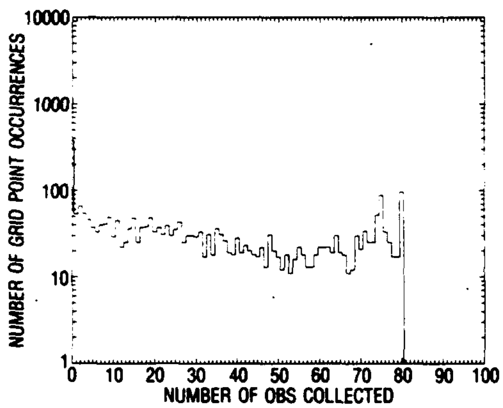

Figure 7. Histogram of all ship and buoy data collected on 14 September 1987. In practice, each grid point was limited to no more than 30 ship and buoy observations. This limit was frequently exceeded.

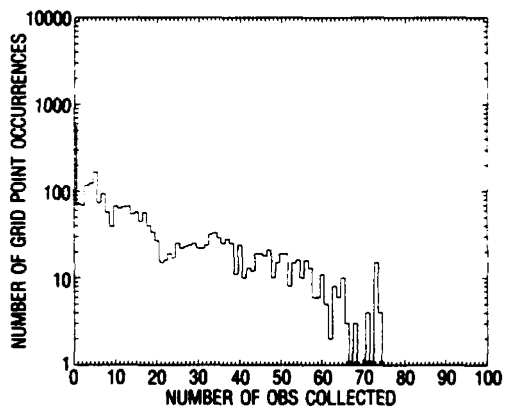

Figure 8. Histogram of all MCSST superob data collected on 14 September 1987. In practice, each grid point was limited to no more than 30 MCSST obs. This limit was frequently exceeded.

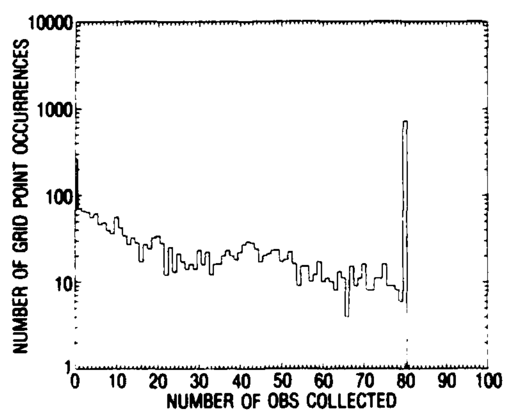

Figure 9. Histogram of all subsurface XBT data collected on 14 September 1987. Each grid point was limited to no more than 80 XBTs, a limit which was frequently encountered.

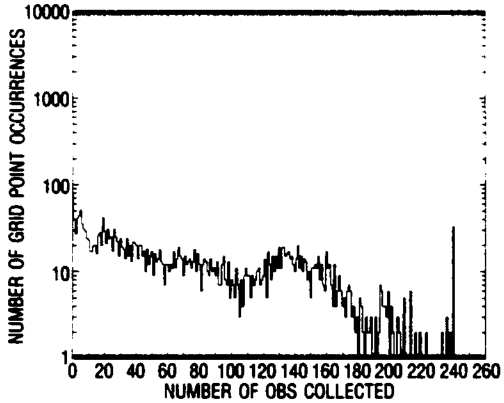

Figure 10. Histogram of all surface data collected on 14 September 1987. Each grid point was limited to no more than 240 observations, a limit that was occasionally exceeded.

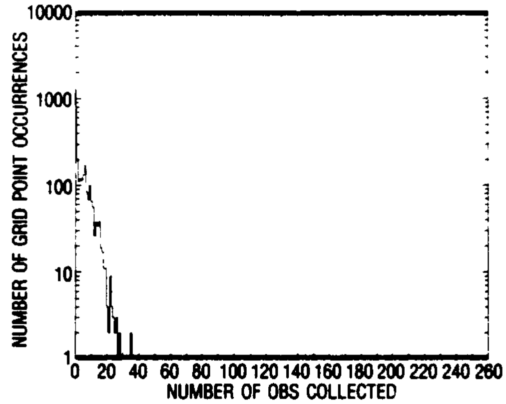

Figure 11. Histogram of XBT SST data collected on 14 September 1987. Note that over 1000 grid points found no XBTs within their search areas.

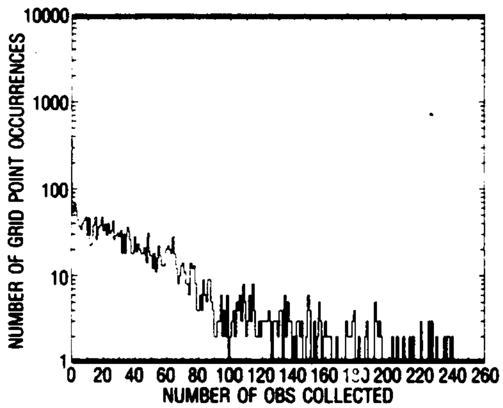

Figure 12. Histogram of ship and buoy data collected on 14 September 1987. Each grid point was limited to no more than 240 total observations.

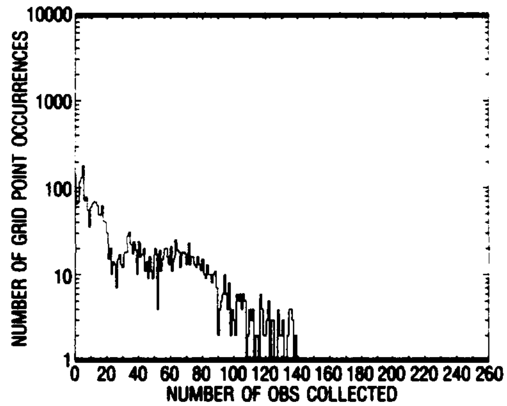

Figure 13. Histogram of MCSST data collected on 14 September 1987. Each grid point was limited to no more than 240 total observations.

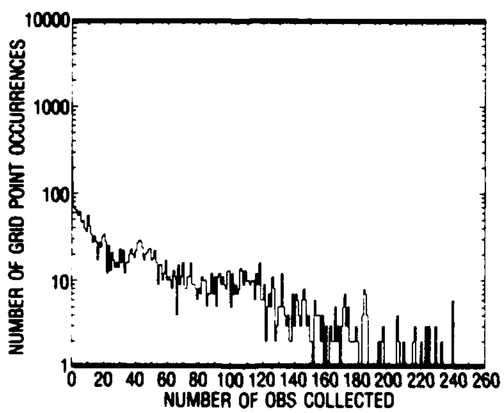

Figure 14. Histogram of subsurface data collected on 14 September 1987. Each grid point was limited to no more than 240 XBTs, a limit that was rarely encountered.

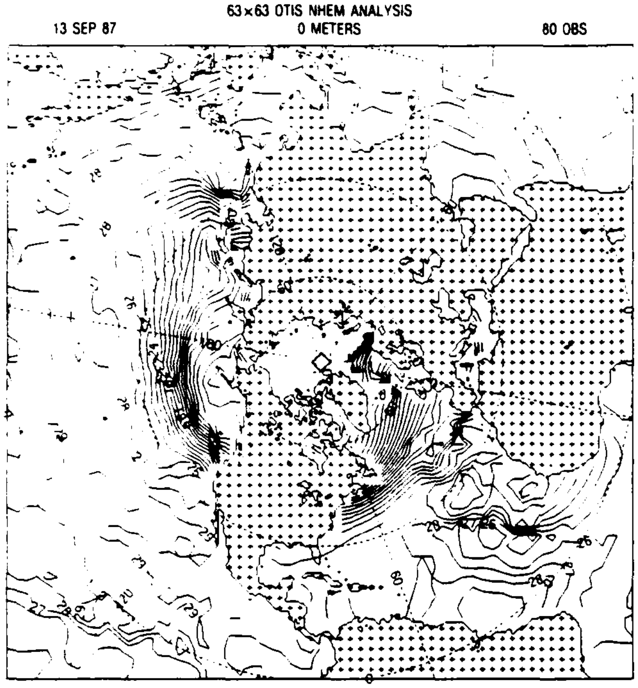

Figure 15. Sea surface temperature analysis resulting from limiting the data collection to no more than 80 observations per grid point.

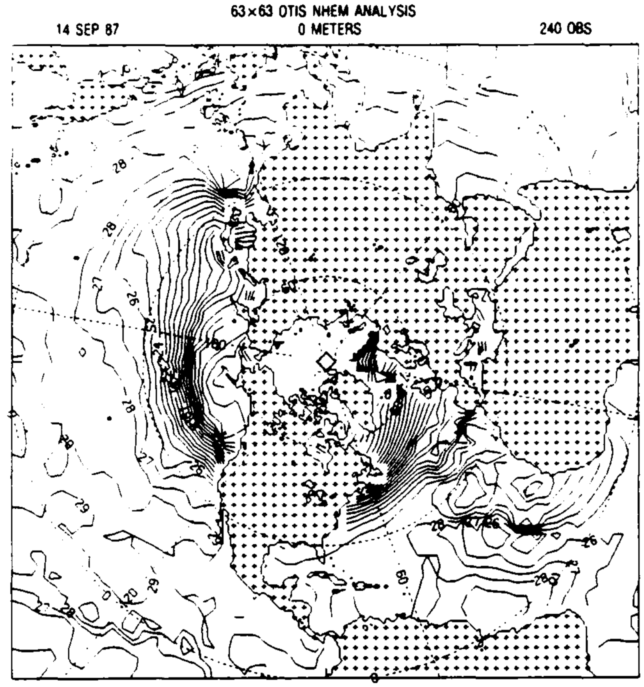

Figure 16. Sea surface temperature analysis resulting from allowing each grid point to collect up to 240 observations.

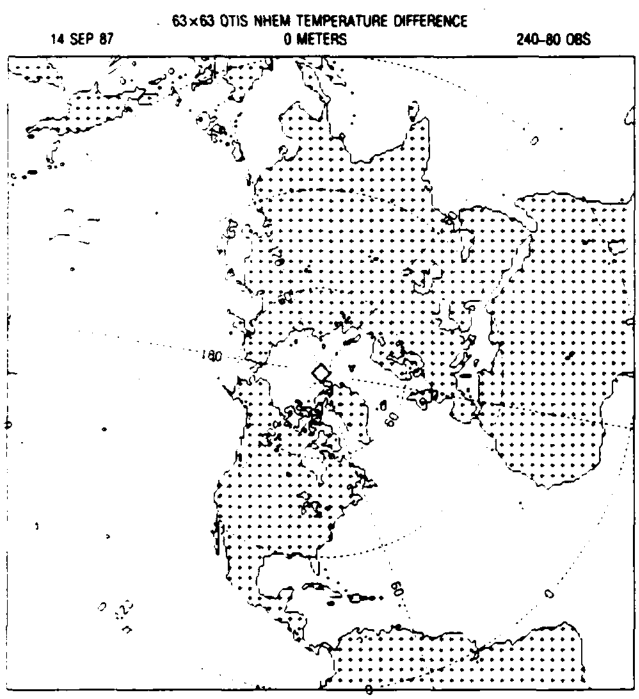

Figure 17. Areas where collecting 240 observations per point, rather than 80, resulted in at least a 0.5° C increase in sea surface temperature.

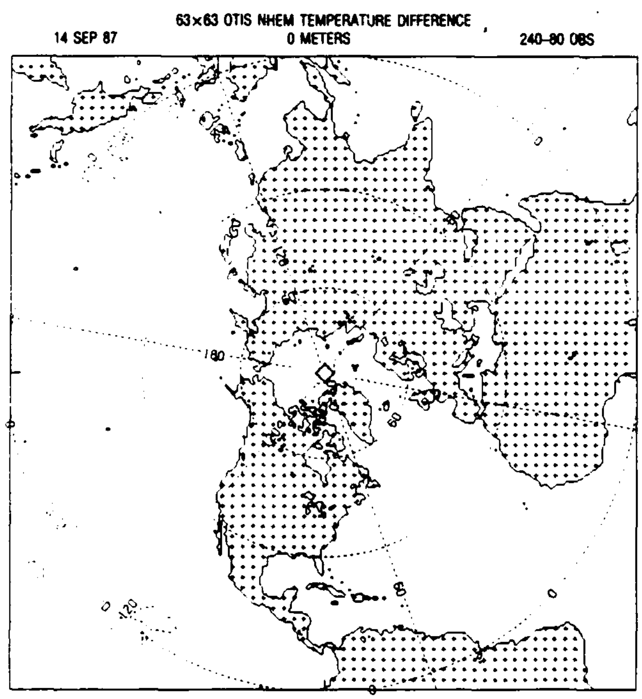

Figure 18. Areas where collecting 240 observations per point, rather than 80, resulted in at least a 0.5° C decrease in sea surface temperature.

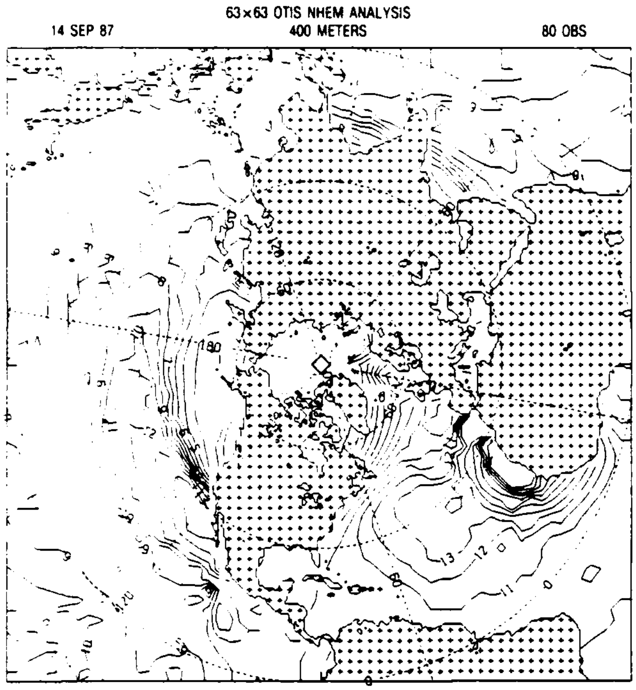

Figure 19. The 400-m temperature analysis resulting from limiting the data collection to no more than 80 observations per grid point.

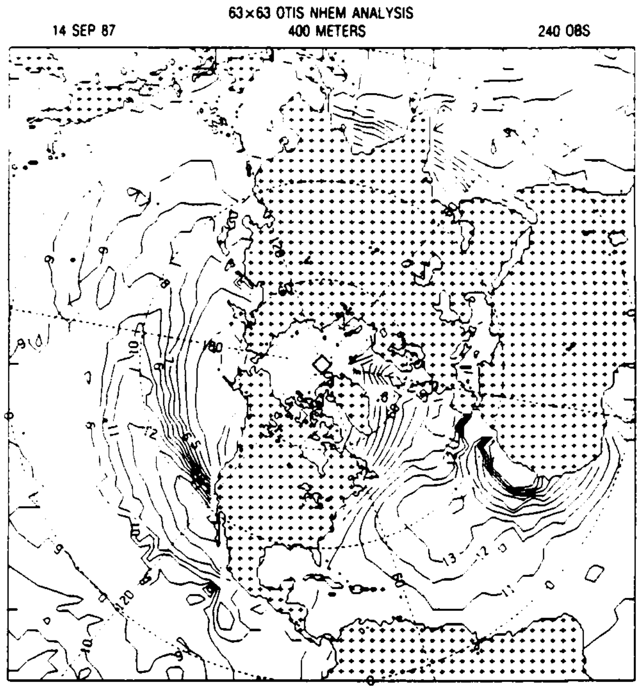

Figure 20. The 400-m temperature analysis resulting from allowing each grid point to collect up to 240 observations.

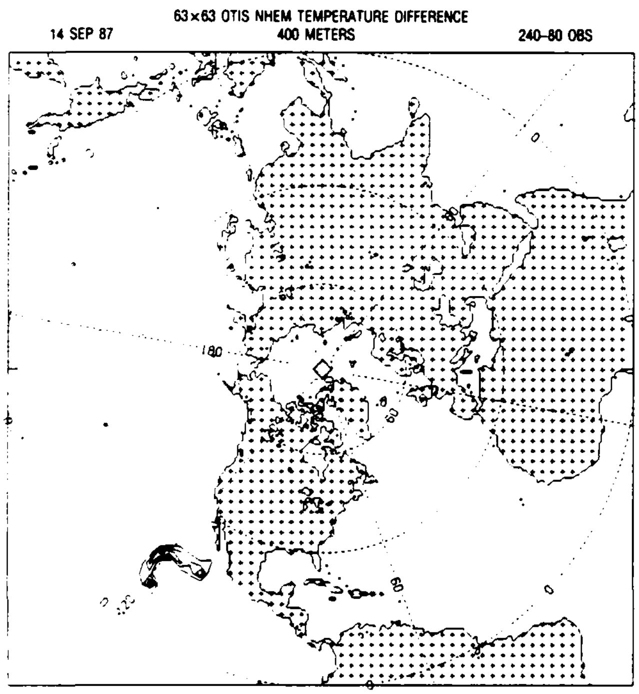

Figure 21. Areas where collecting 240 observations per point, rather than 80, resulted in at least a 0.5° C increase in the 400-m temperature.

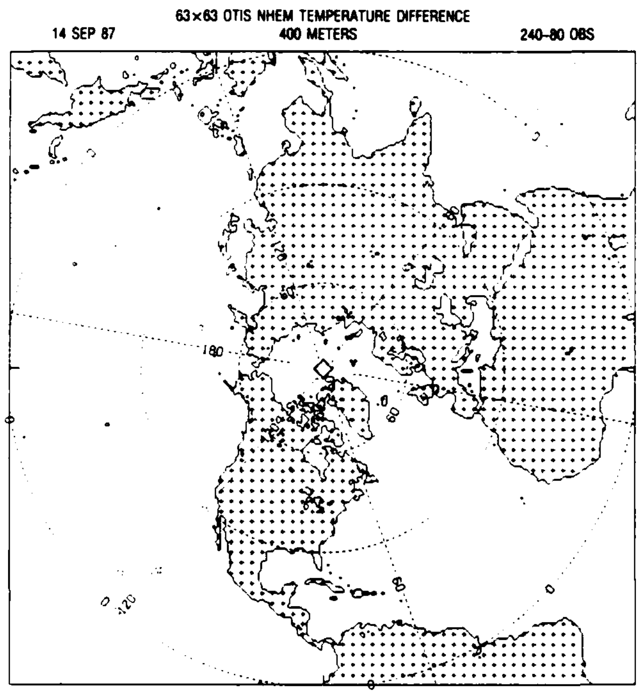

Figure 22. Areas where collecting 240 observations per point, rather than 80, resulted in at least a 0.5° C decrease in the 400-m temperature.

Table 2. Spatial correlation scales used for the OTIS Northern Hemisphere analysis. Scales are in kilometers and are defined for 10 degree latitude by 20 degree longitude boxes, centered at the latitudes and longitudes shown. In practice, any scale smaller than the grid resolution is reset to equal one grid space.

East-West Correlation Scales for OTIS NHEM in km

Latitude	360°W	340°W	320°W	300°W	280°W	260°W	240°W	220°W	200°W
75°N	500	500	100	100	100	10	100	100	100
65°N	500	100	20	10	10	10	10	10	10
55°N	100	10	10	10	10	10	10	250	500
45°N	100	10	10	10	10	10	10	250	500
35°N	100	50	50	10	10	10	250	250	250
25°N	10	10	10	100	10	10	250	1000	1000
15°N	10	10	10	1000	200	100	200	1500	1500
5°N	500	10	100	1500	1500	250	200	2000	2000

Latitude	180°W	160°W	140°W	120°W	100°W	80°W	60°W	40°W	20°W
75°N	100	100	100	10	10	10	500	10	250
65°N	100	10	10	10	10	10	500	500	250
55°N	500	100	100	10	10	10	500	750	750
45°N	750	1000	750	100	10	50	200	500	1000
35°N	1000	1000	750	200	10	100	1000	750	750
25°N	1000	1000	1000	750	100	200	500	1000	500
15°N	1500	1500	1500	1500	1000	200	750	1500	250
5°N	2000	2000	2000	2000	2000	200	100	2000	250

North-South Correlation Scales for OTIS NHEM in km

Latitude	360°W	340°W	320°W	300°W	280°W	260°W	240°W	220°W	200°W
75°N	250	250	100	100	50	10	50	50	50
65°N	250	100	20	10	10	10	10	10	10
55°N	100	10	10	10	10	10	10	100	250
45°N	100	10	10	10	10	10	10	100	100
35°N	100	50	50	10	10	10	200	100	100
25°N	10	10	10	50	10	10	200	500	500
15°N	10	10	10	250	100	100	200	750	750
5°N	200	10	50	750	750	250	200	1000	1000

Latitude	180°W	160°W	140°W	120°W	100°W	80°W	60°W	40°W	20°W
75°N	50	50	50	10	10	10	200	10	200
65°N	50	10	10	10	10	10	200	50	200
55°N	250	50	50	10	10	10	200	200	500
45°N	500	500	500	250	10	50	200	200	500
35°N	500	500	500	250	10	50	100	100	500
25°N	500	500	500	750	100	100	200	500	500
15°N	750	750	750	750	500	100	200	750	750
5°N	1000	1000	1000	1000	1000	100	100	1000	1000

must be done, some way had to be found to reduce the memory requirements of OTIS.

In a cooperative effort between NORDA and FNOC, a scheme was designed which, while simple in principle, would require rewriting major portions of the OTIS software. Rather than collect all the information about each observation found in the search area (latitude, longitude, temperature, age, data type, correlation, identifier, classification, etc.), as was currently being done, only the correlation needed to be saved. Once the correlations of all the collected observations were sorted, and the 15 largest were selected, all that would be needed was a pointer to relocate the selected observations within the large data arrays. The detailed

information could then be unpacked again and saved only for the 15 selected data points. This procedure would greatly reduce the memory requirements and allow the limit on the number of observations to be increased dramatically, without altering any of the principles on which the analysis was based.

As an added benefit, this approach allowed the data selection criteria for the different analysis layers to be further decoupled, so that different correlation scales could be prescribed for the analysis levels above and below 400 m. Before these changes, the XBTs collected for the analyses in the deepest layer were the same as those collected in the layer above 400 m. Now, the data collection is done separately for three layers—the surface, the levels down to 400 m, and the levels below 400 m. If a particular XBT has no data below 400 m, it will not be included in the set of observations collected for the third layer. Because such an XBT will no longer take up space unnecessarily, more room remains for the inclusion of XBTs that actually report data at those lower levels.

These software modifications were developed in NORDA's Remote Sensing Branch and were tested and evaluated in conjunction with FNOC. Because of the need to include the classified XBT data for the operational OTIS, the limit on the number of observations collected had to be further increased. The limit is now set at 700 observations per grid point, and diagnostics that allow monitoring this value for any needed changes have been included. Such monitoring will be essential when data windows or spatial correlation scales are increased, and when regional versions of OTIS are tested.

As a result of the intense scrutiny given to the data during the testing of these corrections, several other errors were discovered. Some of these errors had a significant impact on the data selection. At subsurface, the longitude of the XBT was checked against the latitude bounds of the search area, resulting in subsurface data being erroneously included or excluded. Algorithms for calculating the lowest depth reported in an XBT were wrong; the check for missing levels within an XBT was invalid; variables were left undefined under certain circumstances; satellite data were sometimes interpreted as classified data. Therefore, the modified version of OTIS is more error-free than the original. In addition, OTIS now requires less central memory and runs faster than it did before the data selection algorithms were modified.

VII. Conclusions and Recommendations

In an optimum interpolation analysis system where the analysis proceeds point by point and utilizes only a limited amount of data at each point, certain decisions must be made about that data. It can be thought of as a two-step process—collection and selection. The ultimate goal is to select the data that provide the most useful information about a variable at a given point. Prior to this selection, all of the data in some prescribed area surrounding the grid point are collected. From this data subset, certain observations will be selected for the analysis and others will be excluded. To produce the most realistic analysis, both steps must be carefully executed.

Several problems with the algorithms used for data collection and selection in OTIS have been identified and solutions have been tested. The limits placed on the number of observations that could be collected around a particular grid point were too restrictive. Since the data collection proceeded methodically from south to north, the data most highly correlated with the grid point were frequently excluded and the analyses were possibly biased because of the potential to select most of the data from the region south of the grid point.

The performance of OTIS is monitored by computing the root-mean-square errors in the temperature analyses when compared to independent XBT data at various depths in several different regions of the world's oceans. The areas where the performance of OTIS has been worse than expected are exactly those areas where these changes will have the largest impact—where the spatial correlation scales are large, such as in the tropics and the eastern basins. Statistics must be accumulated over a several-month period before the full impact of these changes can be quantitively demonstrated. Regardless of the outcome, the choice of data cannot be capricious or arbitrary, but must be based on sound ideas, and should include those observations which carry the most pertinent information about the variable being analyzed.

While the analyzed temperature differences observed in these experiments are not dramatic, they are large enough to be significant. Furthermore, if the analysis is coupled with a forecast model, as planned, any errors in the analysis could be expected to grow in the absence of new data. Also, experience with the SST-OTIS indicates that data selection becomes even more critical as the grid resolution decreases and finer-scale features are being analyzed. Therefore, one of the problems that might be encountered in regional versions of OTIS has been circumvented.

As with all systems, there is still room for improvement in these algorithms. Serious thought should be given to increasing the search radius to at least 1.5 times the correlation scale in both directions (Fig. 23). Such an increase would prevent the exclusion of observations that are currently outside the bounds of the data search area, but have correlations with the grid point that are greater than the observations in the corners of the current search area (Fig. 2). Also, by ignoring

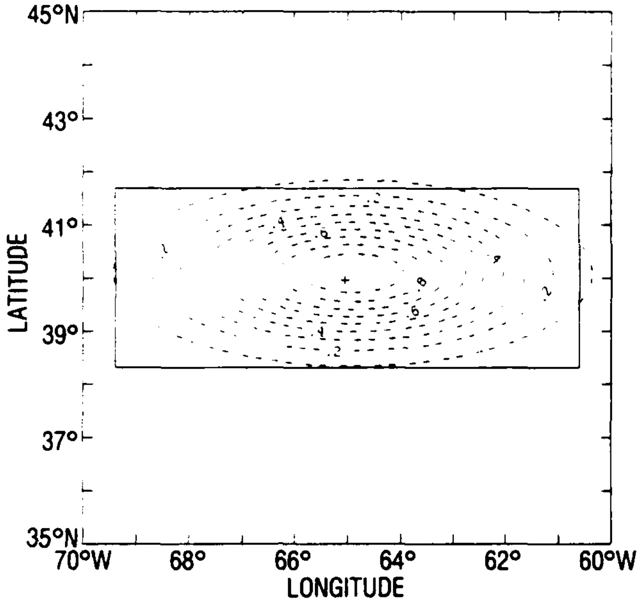

Figure 23. The rectangular area is the area that will be searched for data at this particular grid point, given a search area defined as 1.5 times the correlation length in both the x and y directions from the grid point. The set of concentric ellipses represent the spatial correlation function given an east-west correlation scale of 250 km and a north-south scale of 125 km.

all data with a correlation of less than some small value, say 0.75, the shape of the search area would mimic the shape of the spatial correlation function. Increasing the search area in this way would be more acceptable but would, of course, require more computer resources—resources freed by the improvements resulting from this work.

It would also be interesting to experiment with the number of observations actually used in the analysis at a given point (now a maximum of 15). The current opinion in the meteorological community is that increasing the number of observations has a positive impact (Carr, 1987). By increasing the number of data points influencing the analysis at a point, the grid point method essentially approaches the volume method. OTIS is set up so that the number of observations used can be varied in three possible layers. These layers include the surface, the levels from the base of the mixed layer to 400 m, and the levels below 400 m. Perhaps more data should be used at the surface, where information is more plentiful, and less at subsurface. The cost effectiveness of such modifications would have to be considered. In other words, would there be enough improvement in the analyses to justify the additional computer resources required?

Others (Lorenc, 1981; Phoebus, 1985; DiMego, 1988) have experimented with techniques to prevent selecting data that are highly correlated with one another and that contain redundant information. OTIS, for example, currently filters XBT data to some extent. No more than 15 of the most recent XBT observations are saved within any 2.5 by 2.5 degree latitude/longitude box, with no more than 10 of those reports originating from the same source (SAIC, 1987). Another area where similar changes might be considered is in the treatment of buoy data. Most buoys report temperatures every hour, but their positions have changed little, if at all. Therefore, these data are highly correlated with one another and, at grid points close to the buoy, may completely exclude information from more independent sources. A simple filter to retain only the most recent report from each stationary platform is in use in the SST-OTIS. The same software can also be used to remove duplicate observations from other data sources. Such a filter would be applicable in OTIS, as well, if OTIS were modified so that the various types of buoy data could be distinguished from ship data.

If OTIS is ever transitioned to run operationally on a vector processor, such as the Cyber 205, the volume method (Lorenc, 1981) of selecting and analyzing data would probably be a more appropriate choice. Theoretically, it avoids many of the decisions that must be made when using limited data selection algorithms. Practically, it reduces computer resource requirements by eliminating the repetitive searching through large amounts of data at each grid point to choose only a few. There are other desirable characteristics, such as improved quality control of the input data, which are beyond the scope of this report.

Data selection algorithms can be extremely detailed. As analysis schemes become more complex and more accurate, the data selection and quality control algorithms become perhaps the most important links in the system. The inclusion or omission of even one critical observation can have a significant impact on the resulting analysis (Thiebaux, 1980; Hollingsworth et al., 1985). More and more attention is being paid to such details; they are certainly valid research areas and should be carefully scrutinized in any analysis system.

VIII. References

Alaka, M. A. and R. Elvander (1972). Optimum interpolation from observations of mixed quality. *Monthly Weather Review* 100:612-624.

Baker, W. E., S. Bloom, J. Woolen, M. Nestler, E. Brin, T. Sclatter, and G. Branstator (1987). Experiments with a three-dimensional statistical objective analysis scheme using FGGE data. *Monthly Weather Review* 115:272-296.

Barker, E. H. and T. Rosmond (1985). Short course on objective data analysis and vector computers. *Bulletin of the American Meteorological Society* 66:1153-1157.

Barker, E. H., J. Goerss, and N. Baker (1988). Navy's operational multivariate optimum interpolation

method. Presented at the *Eighth Conference on Numerical Weather Prediction*, February 22-26, 1988, Baltimore, MD.

Bergman, K. (1979). Multivariate analysis of temperature and winds using optimum interpolation. *Monthly Weather Review* 107:1423-1444.

Bretherton, F. P., R. Davis, and C. Fandry (1976). A technique for objective analysis and design of oceanographic experiments applied to MODE-73. *Deep-Sea Research* 23:559-582.

Carr, E. L. (1987). Objective data analysis conference. *Bulletin of the American Meteorological Society* 68:481-484.

Carter, E. F. and A. Robinson (1981). Analysis models for the estimation of oceanic fields. *Journal of Atmospheric and Oceanic Technology* 4:49-74.

Clancy, R. M., K. Pollak, J. Cummings, P. Phoebus (1988). *Technical Description of the Optimum Thermal Interpolation System (OTIS) Version 1: A Model for Oceanographic Data Assimilation*. Fleet Numerical Oceanography Center, Code 42, Monterey, CA 93943, Tech Note 422-86-02 80 pp.

Daley, R., A. Hollingsworth, J. Ploshay, K. Miyakoda, W. Baker, E. Kalnay, C. Dey, T. Krishnamurti, and E. Barker (1985). Objective analysis and assimilation techniques used for the production of FGGE IIIb analyses. *Bulletin of the American Meteorological Society* 77:532-538.

DiMego, G. J. (1988). The National Meteorological Center regional analysis system. *Monthly Weather Review* 116:977-1000.

Freeland, J. H. and W. Gould (1976). Objective analysis of mesoscale ocean circulation features. *Deep-Sea Research* 23:915-923.

Gandin, L. S. (1963). Objective analysis of meteorological fields. *Gidrometeorologichoskoe Isdatel'stvo*, Leningrad. Translated from Russian, Israel Program for Scientific Translations, Jerusalem, 1964, 242 pp.

Hollingsworth, A., A. Lorenc, M. Tracton, K. Arpe, G. Cats, S. Uppala, and P. Kallberg (1985). The response of numerical weather prediction systems to FGGE level IIb data. Part I: Analyses. *Quarterly Journal of the Royal Meteorological Society* 111:1-66.

Lorenc, A. C. (1981). A global three-dimensional multivariate statistical interpolation scheme. *Monthly Weather Review* 109:701-721.

McPherson, R. D., K. Bergman, R. Kistler, G. Rasch, and D. Gordon (1979). The NMC operational global data assimilation system. *Monthly Weather Review* 107:1445-1461.

McPherson, R. D. (1980). *Theory of Optimum Interpolation*. NOAA/NWS/NMC Office Note 217, available from the National Meteorological Center, W/NMC2, WWB, Room 204, Washington, DC 20233.

McWilliams, J. C., W. Owens, and L. Hua (1986). An objective analysis of the POLYMODE local dynamics experiment. Part I: General formalism and statistical model selection. *Journal of Physical Oceanography* 16:483-504.

Phoebus, P. A. (1988). *Improvements to the Quality Control Algorithms in the Optimum Thermal Interpolation System (OTIS)*. Naval Ocean Research and Development Activity, Stennis Space Center, MS, NORDA Report (in prep.).

Phoebus, P. A. (1985). *Data Selection in the NMC Global OI Analysis*. NMC Medium-Range Modeling Branch Paper No. 6, available from the National Meteorological Center, W/NMC2, WWB Room 204, Washington, DC 20233.

Robinson, A. R. and W. Leslie (1985). Estimation and prediction of oceanic eddy fields. *Progress in Oceanography* 14:485-510.

Roemmich, D. (1983). Optimal estimation of hydrographic station data and derived fields. *Journal of Physical Oceanography* 13:1544-1549.

Rutherford, I. D. (1976). An operational three-dimensional multivariate statistical objective analysis scheme. *Proceedings of the Study Group Conference on Four-Dimensional Data Assimilation*, Paris, 17-21 November 1975, GARP Report No. 11.

SAIC (1987). *Users Manual for the Optimum Thermal Interpolation System (OTIS)*. Available from Fleet Numerical Oceanography Center, Monterey, CA 93943.

Schlatter, T. (1975). Some experiments with a multivariate statistical objective analysis scheme. *Monthly Weather Review* 103:246-257.

STX (1987). *Upgrades to OTIS*. ST Systems Corporation (STX), 1900 Garden Road, Suite 130, Monterey, CA 93940, Technical Report STI 6617, 80 pp.

Thiebaux, H. J. (1980). Anticipated changes in analysis accuracy with removal of Ocean Weather Ship P. *Atmosphere-Ocean* 18:261-285.

White, W. B. (1977). Secular variability in the baroclinic structure of the interior North Pacific from 1950-1970. *Journal of Marine Research* 4:587-607.

REPORT DOCUMENTATION PAGE

1a. REPORT SECURITY CLASSIFICATION Unclassified	1b. RESTRICTIVE MARKINGS None
2a. SECURITY CLASSIFICATION AUTHORITY	3. DISTRIBUTION/AVAILABILITY OF REPORT Approved for public release; distribution is unlimited.
2b. DECLASSIFICATION/DOWNGRADING SCHEDULE	
4. PERFORMING ORGANIZATION REPORT NUMBER(S) NORDA Report 239	5. MONITORING ORGANIZATION REPORT NUMBER(S) NORDA Report 239
6. NAME OF PERFORMING ORGANIZATION Naval Ocean Research and Development Activity	7a. NAME OF MONITORING ORGANIZATION Naval Ocean Research and Development Activity
6c. ADDRESS (City, State, and ZIP Code) Ocean Science Directorate Stennis Space Center, Mississippi 39529-5004	7b. ADDRESS (City, State, and ZIP Code) Ocean Science Directorate Stennis Space Center, Mississippi 39529-5004
8a. NAME OF FUNDING/SPONSORING ORGANIZATION Naval Ocean Research and Development Activity 8b. OFFICE SYMBOL (If applicable)	9. PROCUREMENT INSTRUMENT IDENTIFICATION NUMBER
8c. ADDRESS (City, State, and ZIP Code) Ocean Science Directorate Stennis Space Center, Mississippi 39529-5004	10. SOURCE OF FUNDING NOS.

PROGRAM ELEMENT NO.	PROJECT NO.	TASK NO.	WORK UNIT NO.
63704N	0101	100	93217F
63207N	W0513	W0513-CC00	93227C

11. TITLE (Include Security Classification)
Improvements to the Data Selection Algorithms in the Optimum Thermal Interpolation System (OTIS)

12. PERSONAL AUTHOR(S)
Patricia A. Phoebus

13a. TYPE OF REPORT	13b. TIME COVERED	14. DATE OF REPORT (Yr., Mo., Day)	15. PAGE COUNT
Final	From ______ To ______	August 1988	18

16. SUPPLEMENTARY NOTATION

17. COSATI CODES		
FIELD	GROUP	SUB. GR.

18. SUBJECT TERMS (Continue on reverse if necessary and identify by block number)
Optimum Interpolation, SST Analysis, Data Assimilation, Ocean Thermal Analysis, Data Analysis

19. ABSTRACT (Continue on reverse if necessary and identify by block number)
The Fleet Numerical Oceanography Center (FNOC) provides daily analyses of the three-dimensional ocean thermal structure both to the Fleet and to regional naval oceanography centers around the world. These analyses are made for both global and regional areas at resolutions as small as 20 km in some regions. FNOC is planning to update these products very soon with an improved analysis based on the widely accepted methodology of optimum interpolation. This system, the Optimum Interpolation Analysis System (OTIS), is expected to provide a more accurate representation of the three-dimensional ocean thermal structure.

As with any new system, extensive development, testing, and evaluation has been done. Many modifications were made to the original design. While studying the impact of multichannel sea surface temperature data on the analysis of the ocean's sea surface temperature, several errors were uncovered in the data selection algorithms. These errors were also apparent in the subsurface analyses.

Since it is not feasible to use all observations to estimate the temperature at any one location, optimum interpolation chooses a subset of the available data using correlation scales that are representative of the spatial and temporal scales of the ocean features to be analyzed. Practically speaking, observations that are closer to the analysis point and that were taken more recently are the observations most highly correlated with the analysis point.

Generally, all data within a certain cutoff correlation range are collected at an analysis point. Within OTIS, the designated search area was too small and did not correspond to the shape of the spatial correlation function. As a result, observations more highly correlated than those actually collected were excluded from consideration. Furthermore, limited computer resources forced artificial cutoffs to be placed on the collection of observations. The method of data storage resulted in frequently excluding data that were the most highly correlated with the analysis point, while gathering observations farther to the south.

From the initial set of collected data, a few of the most highly correlated reports will be selected as input to the analysis. Only these selected observations will have any effect on the analyzed temperature at that particular location. If the set of collected data does not include the most highly correlated observations, then the selection process cannot choose the most appropriate data for the analysis. Also, if the selected observations are skewed to the south, then biases in the resulting temperature analyses can be produced.

Errors in the data selection procedure were corrected; at the same time the data selection software was redesigned to make more efficient use of the available resources. Correctly selecting the optimum data for the analysis at each point resulted in significant changes in the analyzed temperature fields, and noticeable improvements in the representation of the three-dimensional thermal structure of the ocean.

20. DISTRIBUTION/AVAILABILITY OF ABSTRACT UNCLASSIFIED/UNLIMITED ☐ SAME AS RPT. ■ DTIC USERS ☐	21. ABSTRACT SECURITY CLASSIFICATION Unclassified

22a. NAME OF RESPONSIBLE INDIVIDUAL	22b. TELEPHONE NUMBER (Include Area Code)	22c. OFFICE SYMBOL
Patricia A. Phoebus	(601) 688-5452	Code 321